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Contents

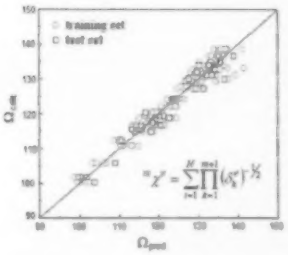
Regular Article

1–5

Prediction of peptide IMS cross sections from extended molecular connectivity

Alexander A. Oliferenko, Feifei Tian, Mati Karelson, Alan R. Katritzky

► Molecular connectivity significantly controls peptide IMS cross-section. ► Topological indices based on extended connectivity provide excellent one-parameter correlations with IMS cross-section oftripeptides. ► Second order valence connectivity index $^{2}\chi^{v}$ is particularly relevant because it encodes tri-atomic peptide fragments.

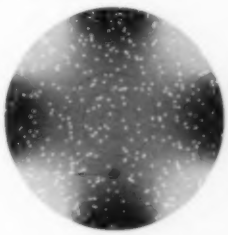


6–12

A study of octupolar excitation for mass-selective centering in Penning traps

M. Rosenbusch, Ch. Böhm, Ch. Borgmann, M. Breitenfeldt, A. Herlert, M. Kowalska, S. Kreim, G. Marx, S. Naimi, D. Neidherr, R. Schneider, L. Schweikhard

► We investigate the applicability of octupolar excitation in buffer-gas filled Penning traps. ► The experiment yields a drop of resolving power for octupolar excitation as compared to the expectations. ► A simulation including ion-atom collisions has been written in order to explain the measurements. ► The simulation shows a crucial influence of the buffer-gas on the ion trajectory during octupolar excitation.

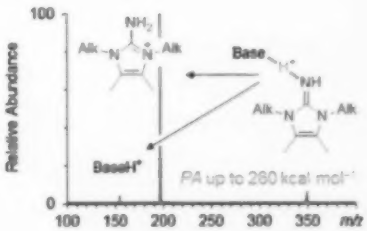


13–17

Proton affinities of 2-iminoimidazolines with bulky *N*-alkyl-substituents

Svetlana M. Polyakova, Roman A. Kunetskiy, Detlef Schröder

► The fragmentation patterns of sterically crowded 2-iminoimidazolines have been measured. ► The proton affinities of these 2-iminoimidazolines have been determined experimentally. ► The normal and the extended kinetic method have been used. ► The experimental data are supported by DFT calculations of the proton affinities. ► A phosphazene base is used as an independent reference.



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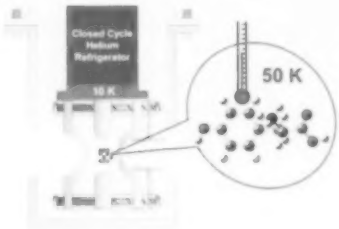
18–21

Effective temperature of protonated tyrosine ions in a cold quadrupole ion trap

Chang Min Choi, Dae Ho Choi, Nam Joon Kim, Jiyoung Heo

► We measured the effective temperatures of protonated tyrosine ions stored in the quadrupole ion trap at ~10 K using laser spectroscopic techniques. ► The rotational temperature was estimated to be 45–54 K from the rotational band contour analysis, showing dependence on the buffer-gas pressure inside the ion trap. ► The rise of the rotational temperature with increasing the buffer-gas pressure was observed. ► The vibrational temperature was determined to be 50 K from the relative intensity of a hot vibronic band, taking its Franck–Condon factor into account.

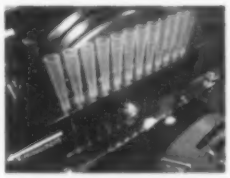


22–32

Assessing the capabilities of direct analysis in real time mass spectrometry for 5-hydroxymethylfurfural quantitation in honey

Elena S. Chernetsova, Gertrud E. Morlock

► Limitations of direct analysis in real time mass spectrometry (DART-MS). ► Influence of instrumental parameters on mass spectra for 5-hydroxymethylfurfural (HMF) and carbohydrates. ► Carbohydrate degradation in DART-MS. ► DART-MS screening of honey for HMF. ► First data on scanning surface analysis with DART-MS.

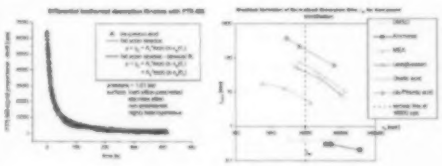


33–41

Desorption kinetics with PTR-MS: Isothermal differential desorption kinetics from a heterogeneous inlet surface at ambient pressure and a new concept for compound identification

Erna Schuhfried, Eugenio Aprea, Luca Cappellin, Christos Soukoulis, Roberto Viola, Tilmann D. Märk, Flavia Gasperi, Franco Biasioli

► We investigate data from differential isothermal desorption kinetics with PTR-MS. ► We quantify highly heterogeneous inlet surface kinetics at ambient pressure. ► We identify a pseudo 1st order bimodal kinetics and log–log linear isotherms. ► Development of a quasi-initial adsorption concentration independent parameter, t_{rid}. ► New concept for compound identification based on normalized desorption time, t_{rel}.

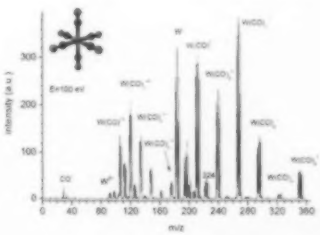


42–48

Electron ionization of $W(CO)_6$: Appearance energies

K. Wnorowski, M. Stano, W. Barszczewska, A. Jówko, Š. Matejčík

► Electron ionization of tungsten hexacarbonyl – $W(CO)_6$. ► Relative cross sections for singly and doubly charged ions. ► Breakdown curves. ► The ionization energies of the molecule and appearance energies of the fragment ions. ► Estimation of bond dissociation energies of the molecular ions.

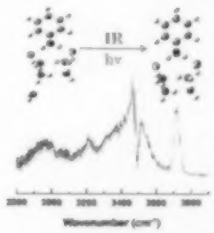


49–56

Infrared photodissociation of aniline$(H_2O)_n^+$ (n = 7–12) clusters

Md. Alauddin, Jae Kyu Song, Seung Min Park

▶ No proton transfer occurs for n = 7–12 clusters. ▶ Multi-ring structures found for n = 7–11 clusters. ▶ A "real" cage-like structure evolved with the increase in cluster size (n = 12).

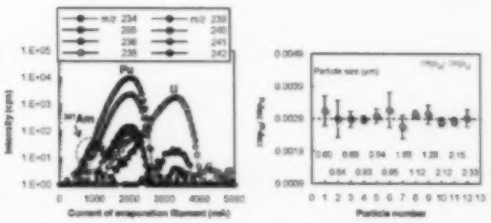


57–62

Simultaneous determination of plutonium and uranium isotope ratios in individual plutonium–uranium mixed particles by thermal ionization mass spectrometry

Chi-Gyu Lee, Daisuke Suzuki, Yoko Saito-Kokubu, Fumitaka Esaka, Masaaki Magara, Takaumi Kimura

▶ MOX (mixed U–Pu oxide) particles were prepared from the mixed solution of plutonium (SRM947) and uranium (U500). ▶ We developed a method for simultaneously measuring all the Pu and U isotopes in MOX particles without chemically separating the sample, using thermal ionization mass spectrometry with a peak-jumping mode. ▶ The accurate measurement of the $^{238}Pu/^{239}Pu$ ratio in MOX particles could be performed by using a fitting method to correct the background of ^{238}U at ^{238}Pu.



Corrigendum

63–63

Corrigendum to "Gas-phase ligand binding to Jacobsen's manganese salen catalyst: Functional group and steric effects" [Int. J. Mass Spectrom. 305 (2011) 40–44]

William C. Clodfelter, Emileigh M. Wong, Kelly A. Hay, Scott Gronert